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Ion channeling studies for the determination of orientation of the epilayers in an ion-beam-synthesized $Si/CoSi_2/Si(111)$ system

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Abstract : The orientation of the top Si and the buried $CoSi_2$ epitaxial layers in an ion-beam-synthesized epitaxial $Si/CoSi_2/Si(111)$ system has been determined with Rutherford backscattering spectrometry and channeling techniques using 1.0 MeV He^+ ions. The off-normal axial channeling studies at and around the [110] and the [114] crystallographic directions of the bulk Si have been performed. The results show that both the top Si layer (88 nm) and the buried $CoSi_2$ layer (68 nm) have the same orientation (type-A) as the bulk Si underneath

Keywords : Epitaxial layer, Rutherford backscattering spectrometry, channeling, epilayer orientation
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1. Introduction

The formation of epitaxial $CoSi_2$ films on a silicon substrate has received much attention in recent years in fundamental studies as well as for possible applications in microelectronic devices such as metal-base and permeable-base transistors [1]. $CoSi_2$ has low resistivity and good thermal stability. The growth of epitaxial $CoSi_2$ on Si has become possible due to its cubic structure and small lattice mismatch (-1.2%) with Si. It has been successfully grown epitaxially on Si under ultrahigh vacuum (UHV) condition. Also a high-dose Co^+ implantation into a silicon substrate and subsequent annealing lead to the growth of a buried $CoSi_2$ epitaxial layer in the Si substrate. The process is known as ion beam synthesis (IBS) [2]. The knowledge of the structural aspects of these epilayers is important for an understanding of the electronic properties. For example, Schottky barrier height at an interface depends on the orientation of the epilayer with respect to that of the substrate [3]. Rutherford backscattering spectrometry (RBS)/channeling, x-ray rocking

curve and x-ray standing wave measurements have been carried out on the ion-beam-synthesized $Si/CoSi_2/Si(111)$ system to determine the crystalline quality [2, 4], the strain in the system [5], the defects and their distribution at the interfaces [6], the interfacial atomic structure [7] and the orientation at interfaces. A detailed report on various aspects of silicides prepared by IBS can be found in reference [2].

There are two possible orientations in which an epitaxial silicide layer can grow: type-A, where the silicide layer has the same orientation as the Si substrate, and type-B (twinned), where the silicide layer is rotated 180^o about the surface normal of the Si substrate [Fig.1].

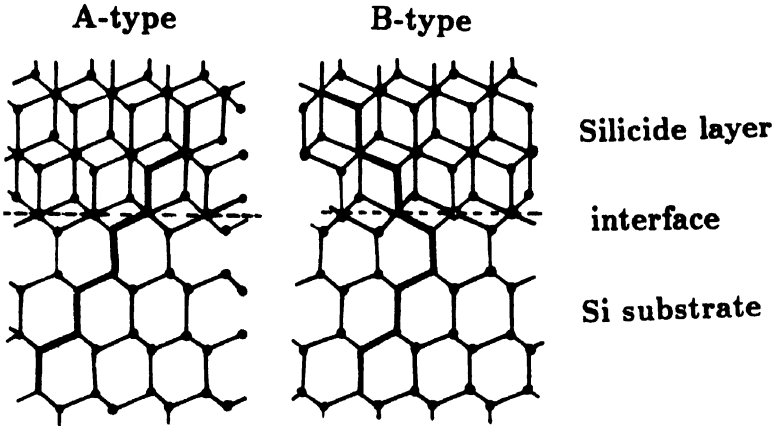

Fig.1 Type-A, where the silicide layer has the same orientation as the Si substrate, and type-B (twinned), where the silicide layer is rotated 180^o about the surface normal of the Si substrate. The dark step-like lines indicate the relative orientations.

For a $CoSi_2$ layer on Si, with the UHV method one can fabricate only a B-type layer, whereas with the IBS method fabrication of both A- and B-type layers is possible. It has been observed that for the IBS-prepared samples, there is a critical thickness (t_c) above which a pure type-A $CoSi_2$ layer can be grown. The critical thickness (t_c) has been found to be 30 nm for the $Si/CoSi_2/Si(111)$ system [8]. Below t_c the layer is usually a mixture of both A- and B-type regions, except for an ultrathin layer where a pure B-type growth is possible. These silicides can form atomically abrupt and structurally perfect Schottky-barrier interfaces. It has been found, both experimentally and theoretically, that the Schottky-barrier heights for A-type and B-type interfaces are different [3]. Thus, a knowledge of the epilayer orientation (whether A-type or B-type) is essential to understand the elctronic properties of these structures. Here we present the determination of the orientation of both the top Si layer and the buried $CoSi_2$ layer in an ion-beam-synthesized $Si/CoSi_2/Si(111)$ system using the RBS/channeling technique.

2. Experimental

The method of sample preparation [2] and the measurement of layer thickness [4] have been discussed elsewhere.

The RBS/channeling measurements with 1.0 MeV He^+ ions have been carried out for determining the orientation of the epilayers in the system. The surface normal is along the common [111] crystallographic axis. The angular scans were performed with the incident beam direction around the [110] direction (which is tilted by 35.26° from the [111] direction) and the [114] direction (which is also tilted by 35.26° from the [111] direction but in the opposite direction to that of the [110] direction) of the substrate (Fig. 2). The details about the experimental setup has been reported elsewhere [4, 9].

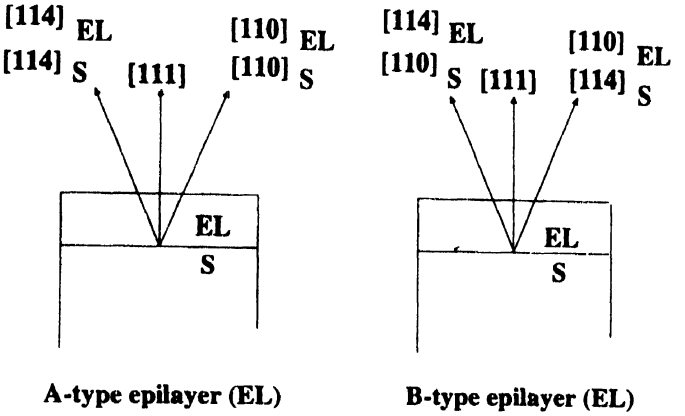

Fig.2 Crystallographic directions in the substrate (S) and the epilayer (EL) are shown. For a *Si* substrate the angle between [111] and [110] (or [114]) directions is 35.26°.

In an usual RBS experiment the incident beam direction is chosen such that it does not coincide with any (specially low index) crystallographic direction of the single crystalline sample; when it does coincide the yield of backscattered ions reduces drastically because under this condition most of the ions are weakly scattered in the forward direction by the atomic strings in the sample and channel into the sample crystal. The degree of reduction depends on the crystallographic directions, as the strength of the scattering depends on them [10]. The reduction in the backscattering yield is usually monitored while scanning the beam direction around a crystallographic axis. This shows gradual reduction from random to the aligned yield [4]. The yield as a function of tilt angle for several crystallographic directions in the diamond (e.g. *Si*) and the CaF_2 (e.g. $CoSi_2$) structure is schematically shown in Fig. 3. We notice that the reduction is much more for the [110] direction compared to the [114] direction. This feature can be used to distinguish between

the [114] and the [110] directions from the measured yield. For our sample, $Si/CoSi_2/Si(111)$, the yields from each layer can be identified in the RBS spectrum, and therefore the yield variation for the top Si, the buried $CoSi_2$ and the bulk Si layer can be individually studied to determine their respective crystallographic orientations. This is what has been done in the present experiment.

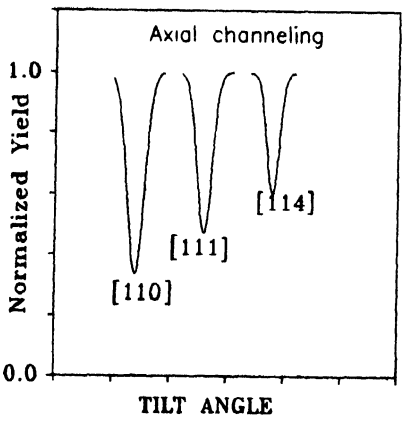

Fig. 3. Schematic representation of the yield as a function of tilt angle for some crystallographic directions in the diamond (e.g. Si) and the CaF_2 (e.g. $CoSi_2$) structure.

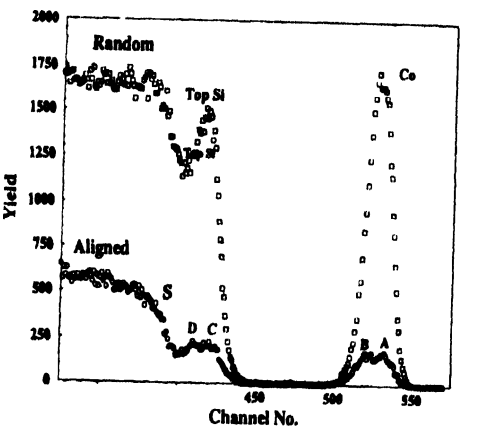

Fig. 4. Typical RBS spectra for the random incidence (◇) and for an aligned incidence (+) (aligned to [111] axis) of the ion beam.

3. Results and discussions

Fig.4 shows typical RBS spectra for the random incidence and for an aligned incidence (aligned to [111] axis) of the ion beam. We notice the drastic reduction in the backscattering yield when all other experimental conditions are preserved except the incident beam direction is aligned with a crystallographic axis of the sample. In this case, all the layers have a common [111] direction. When defects are present at an interface, additional backscattering is produced by these defects which is evident from the various peaks: A, B, C and D. A systematic analysis of these interface peak intensities as a function of incident ion energy has been made to obtain the information about the nature of the interfacial defects and their densities [6]. Reduction in the backscattering yield has been observed along other crystallographic directions as well. Fig. 5. shows the yield variations for the top Si, the buried $CoSi_2$ and the bulk Si layer around the [110] and the [114] direction of the bulk Si. In an angular scan the tilt angle was scanned in steps of 0.1 degree. At each angular position a complete backscattering spectrum has been taken. An energy (channel no.) window has been chosen in three regions representing

three layers. The normalized yield has been obtained by taking the ratio of the backscattering yield in these three regions at a given tilt angle to that at random condition. Fig. 5 shows the variation of the normalized yield in the angular scans.

Let us first concentrate on the results for the bulk Si. The reduction in the yield is more for the dip at $+35.26^{o}$ indicating that this direction is [110]. The shallower dip at -35.26^{o} corresponds to the [114] crystallographic direction. For the $CoSi_2$ layer we notice the same trend – the deeper dip at $+35.26^{o}$ and the shallower dip at -35.26^{o}. This means that the [110] and the [114] crystallographic directions of the $CoSi_2$ layer are aligned with the [110] and the [114] directions of the bulk Si, respectively. That is, the $CoSi_2$ layer is A-type. It is obvious that the top Si epilayer also has the same crystallographic orientation as that of $CoSi_2$ and bulk Si. That is, it is type-A with respect to both the layers underneath. For the $CoSi_2$ layer, our results are in agreement with what is expected from the studies in Ref. [8].

It should be noted here that the [110] ([114]) direction of the $CoSi_2$ layer is not in perfect alignment with the [110] ([114]) direction of the bulk Si. This feature is not very clear in Fig. 5.

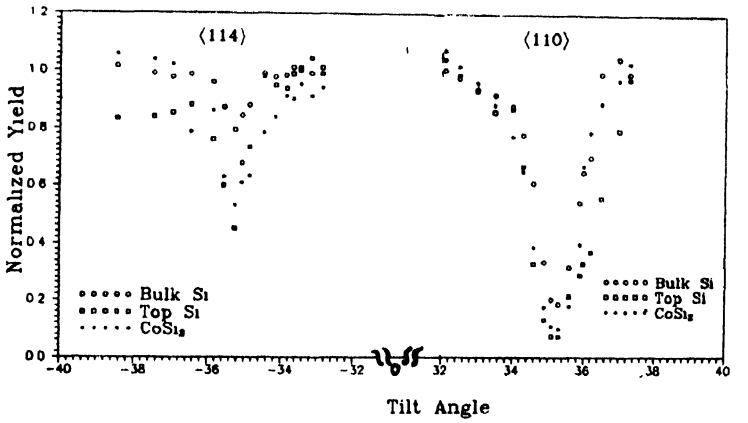

Fig 5. Variation of the normalized yield with tilt angle. The tilt angle is measured with respect to the [111] direction.

At relatively low incident ion energies small misalignments are masked by an ion beam steering effect, which can be avoided by choosing higher energy ions [11]. Measurement of this misalignment angle provides information about the strain in the epitaxial layer. We have made these measurements on the same sample and determined the strain in the $CoSi_2$ layer [12].

The orientation of an epilayer can also be determined by cross-sectional transmission electron microscopy. However, this is a destructive method. On the other hand, the RBS/channeling technique is non-destructive and the

samples can be used for other studies (e.g. electronic properties) after the RBS/channeling characterizations have been made.

4. Conclusions

We have determined the crystallographic orientations of the top Si and the buried $CoSi_2$ epilayers in an IBS-prepared $Si/CoSi_2/Si(111)$ sample using the combined RBS/channeling technique. Both the epilayers have been found to have the same orientation (A-type) as the bulk Si underneath. In the RBS/channeling measurements with an MeV ion beam the penetrating power of MeV ions into solids is effectively exploited to study buried layers in a solid substrate in a non-destructive manner.

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